Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

New Insights into the Mechanical and Self-healing Properties of Polymers Cross-linked by Fe(III)-2,6-pyridinedicarboxamide Coordination Complexes

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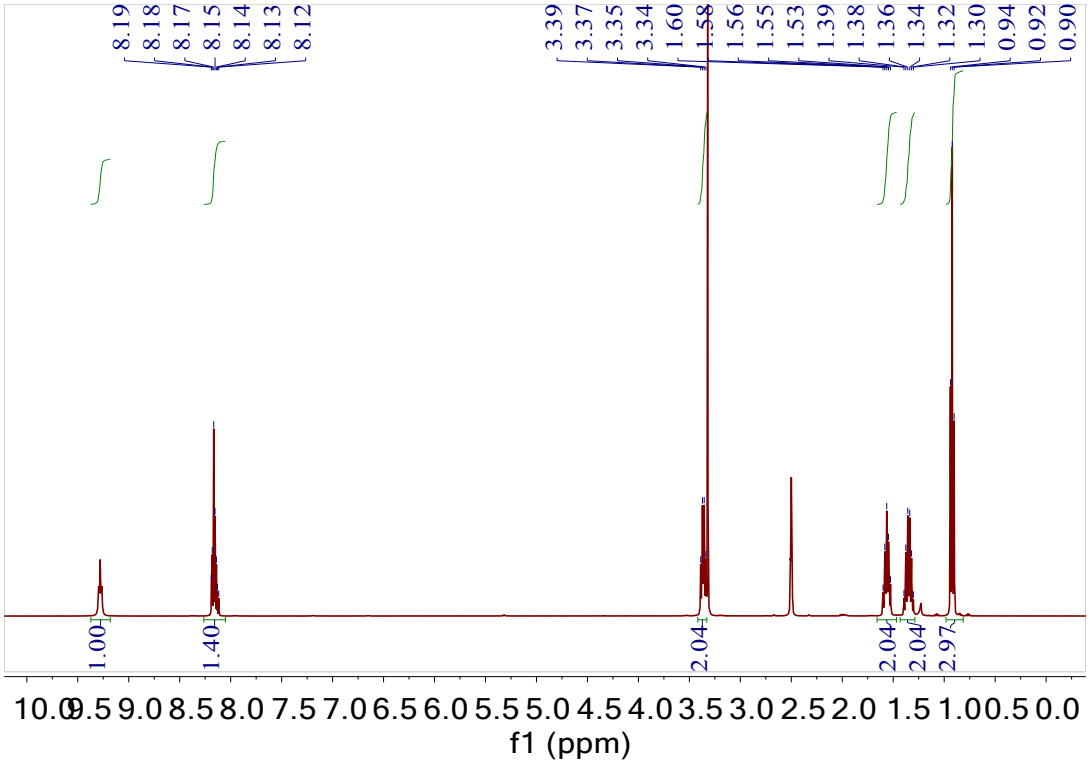

Figure S1. ^{1}H NMR spectrum of compound H_2Bupdca (500 MHz, DMSO–d_6).

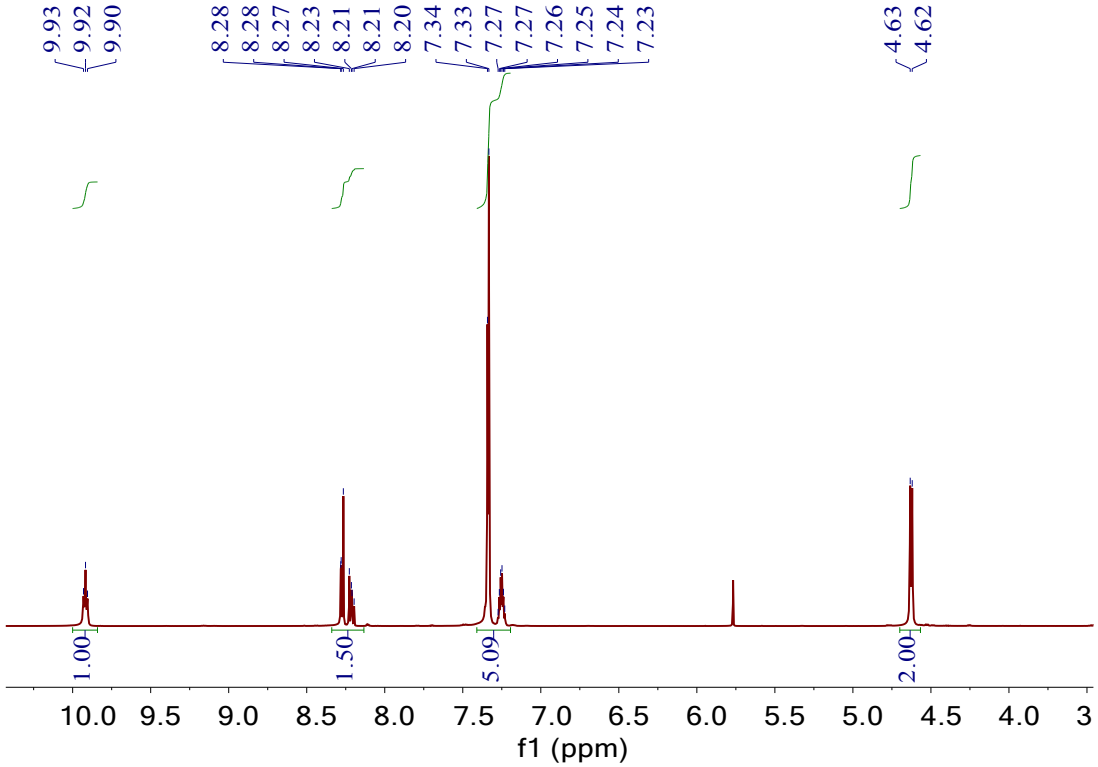

Figure S2. ^{1}H NMR spectrum of compound H_2Bzpdca (500 MHz, DMSO–d_6).

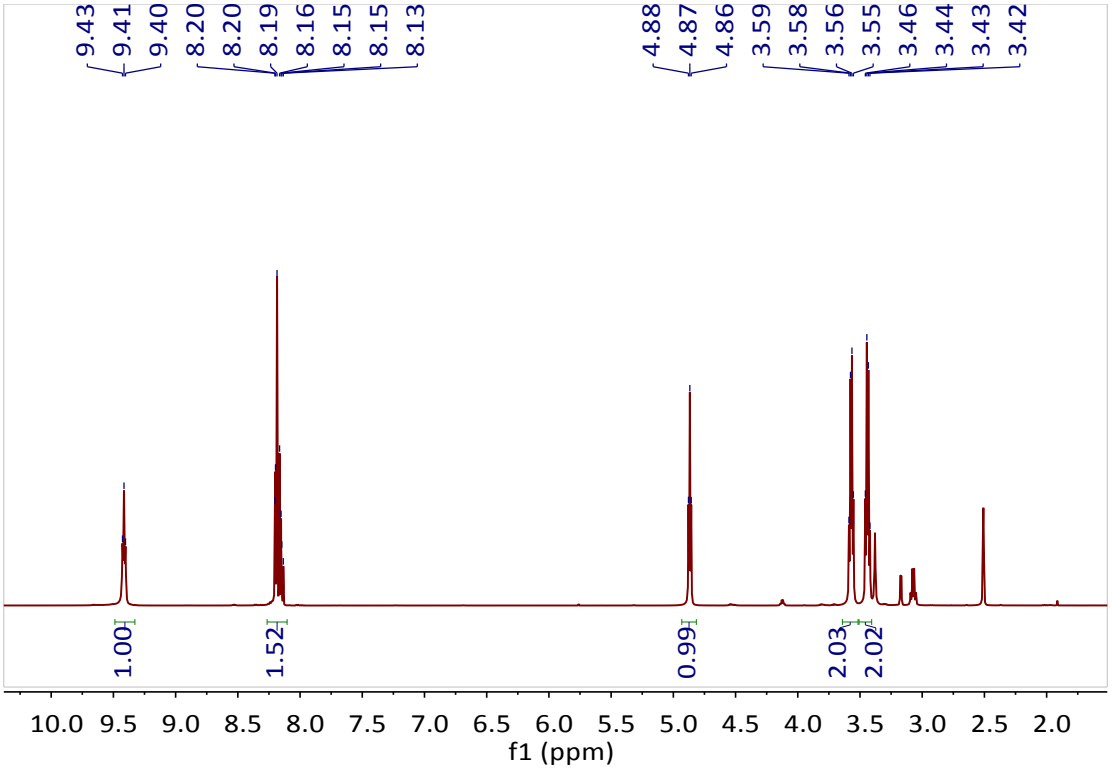

Figure S3. ^{1}H NMR spectrum of compound H_2hepdca (500 MHz, DMSO–d_6).

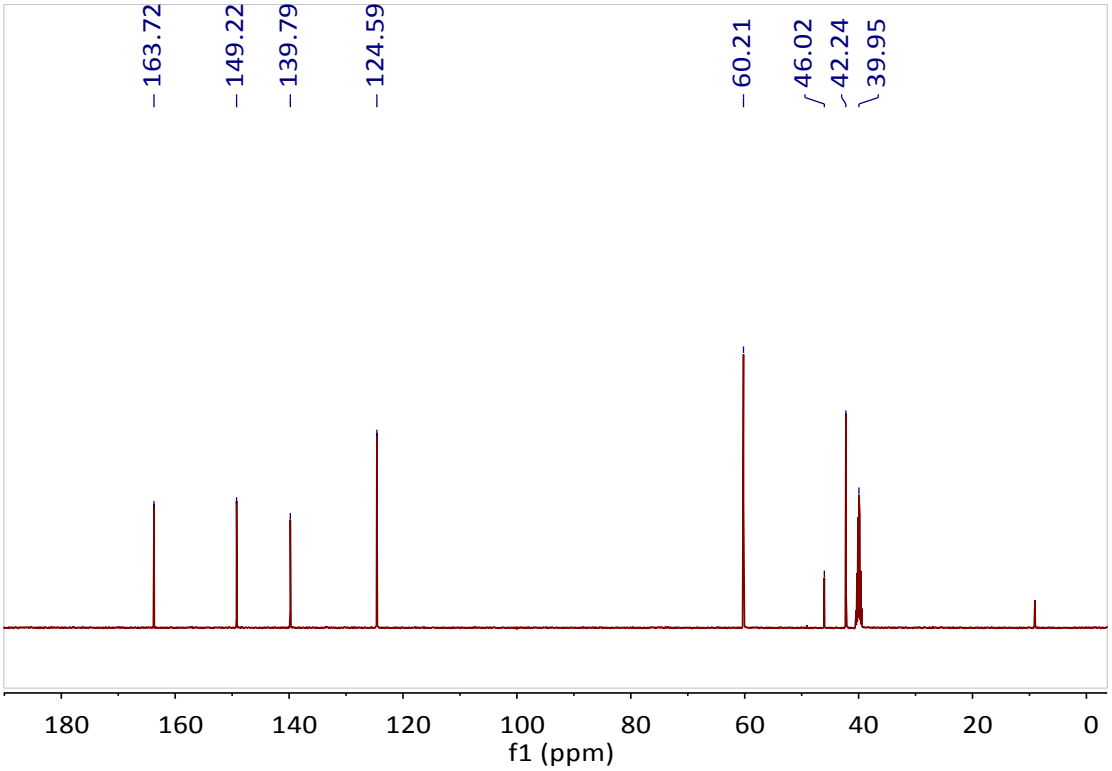

Figure S4. ^{13}C NMR spectrum of compound H_2hepdca (500 MHz, DMSO–d_6).

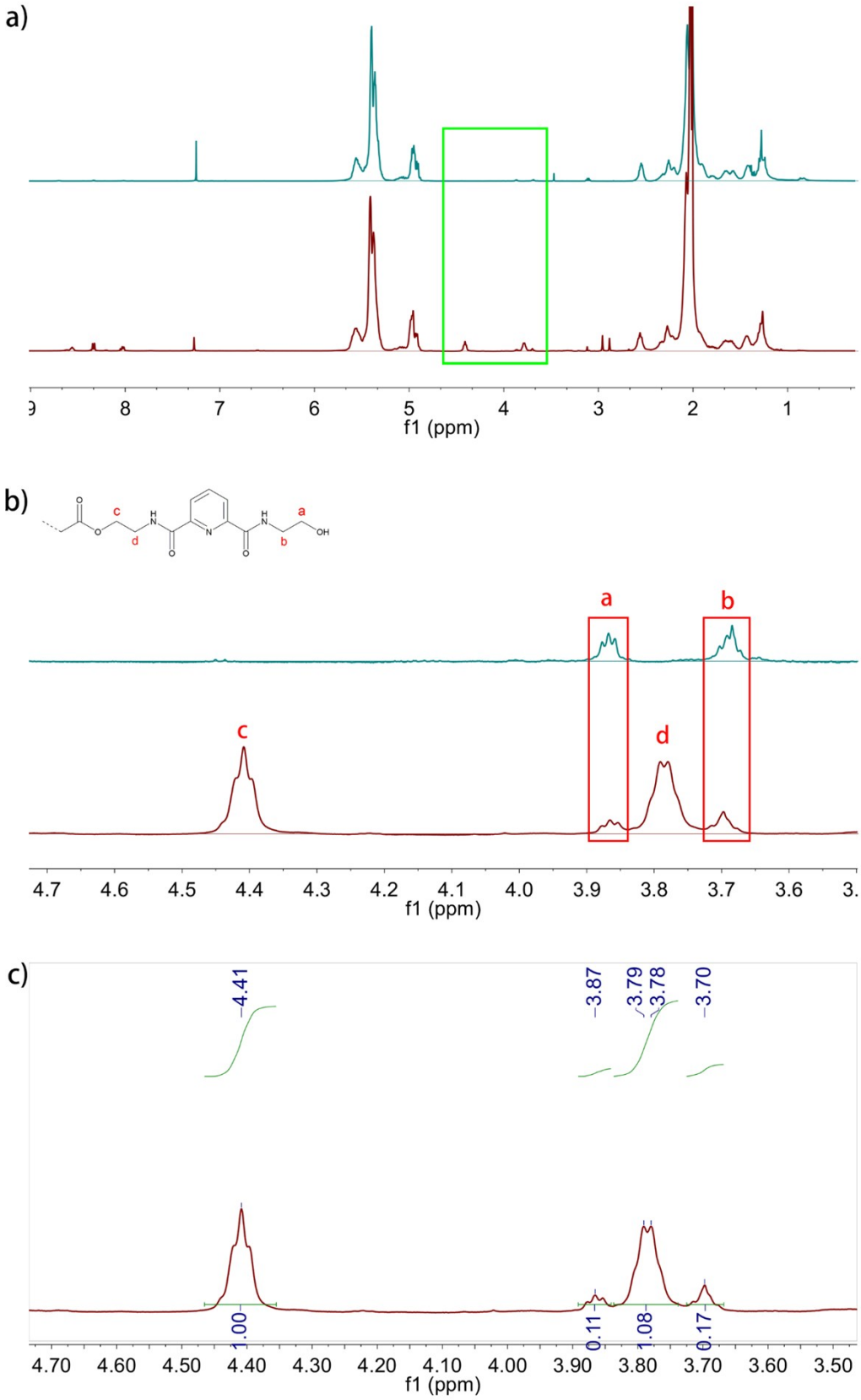

Figure S5. The molecular weight of H_2pdca-PBCA was determinated by ^{1}H NMR (500 MHz, $CDCl_3$). a) ^{1}H NMR spectra of the direct mixture of H_2hepdca and PBCA-COOH without any additions (darkcyan line) and H_2pdca-PBCA (chestnut line). b) Local enlarged drawings of a). c) Local ^{1}H NMR spectrum of

H_2pdca-PBCA. The degree of polymerization = $\frac{1.00}{0.11}$ = 9.1, so the estimated molecular weight = 4000 × 9.1 + 253 × 10 = 61700.

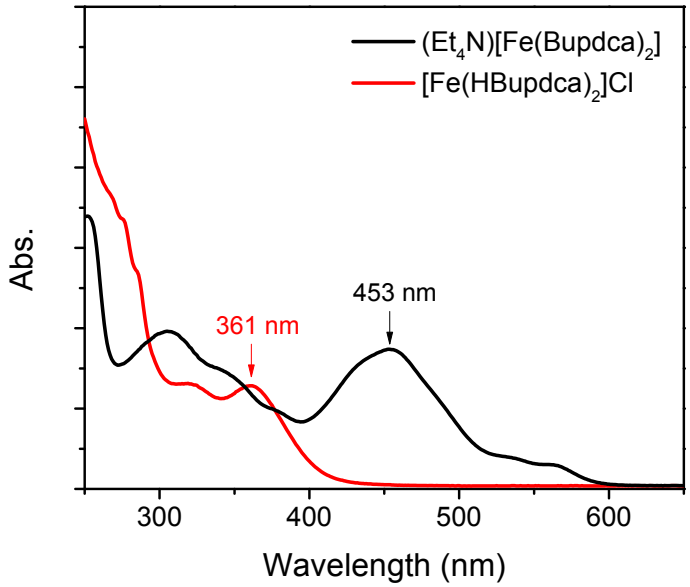

Figure S6. UV–vis spectra of model complexes $Et_4N[Fe(Bupdca)_2]$ and $[Fe(HBupdca)_2]Cl$.

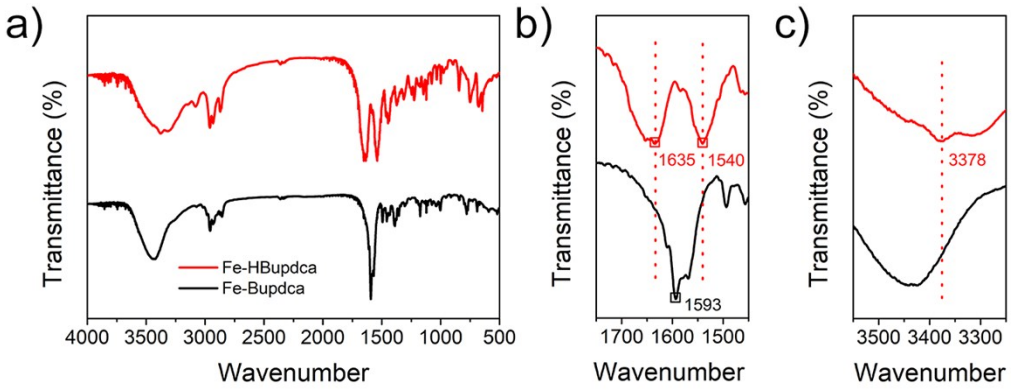

Figure S7. FT-IR spectra of $Et_4N[Fe(Bupdca)_2]$ (black line) and $[Fe(HBupdca)_2]Cl$ (red line) in the range of a) 4000–500 cm^{-1}, b) 1750–1450 cm^{-1} and c) 3550–3250 cm^{-1}.

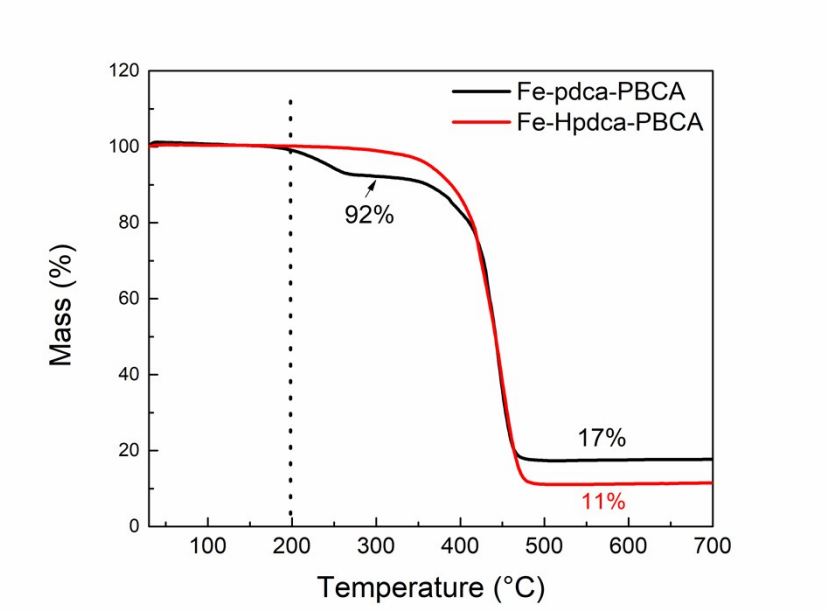

Figure S8. TGA curves of Fe-Hpdca-PBCA and Fe-pdca-PBCA polymers, at a heating rate of 10 °C/min under nitrogen atmosphere.

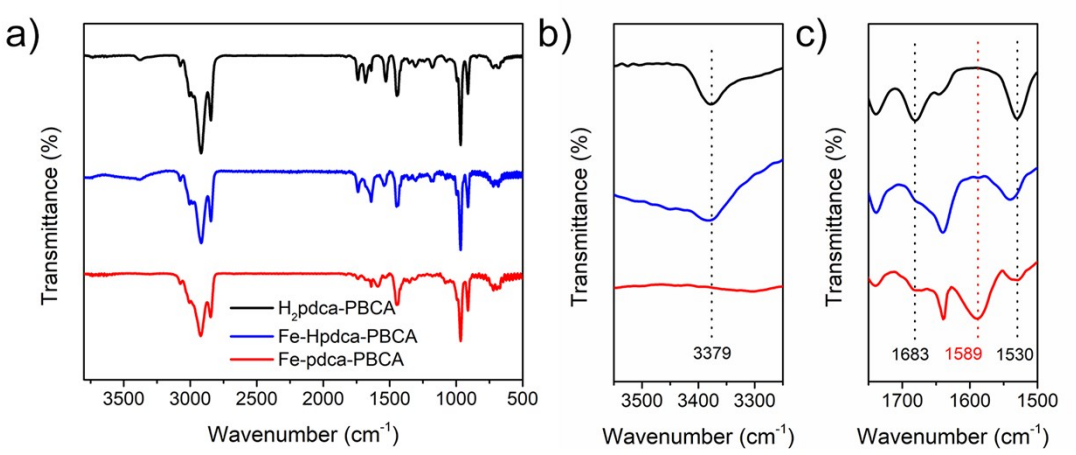

Figure S9. FT-IR spectra of H_2pdca-PBCA (black line), Fe-Hpdca-PBCA (blue line) and Fe-pdca-PBCA (red line) in the range of a) 3800–500 cm^{-1}, b) 3550–3250 cm^{-1} and c) 1750–1500 cm^{-1}.

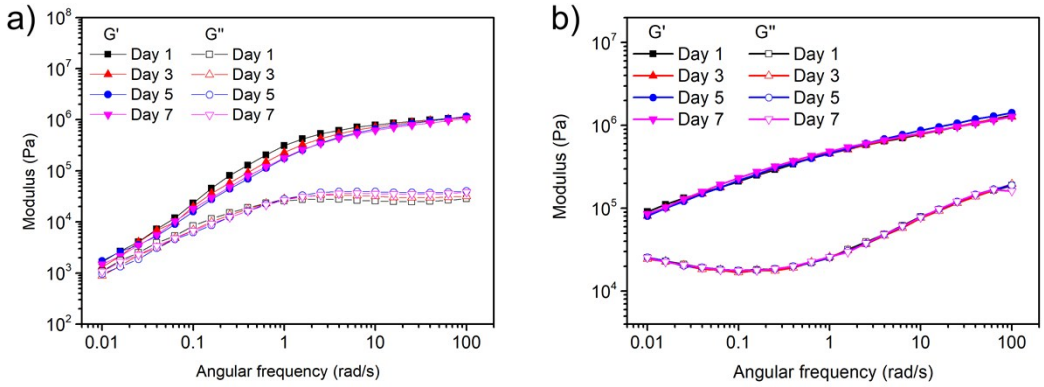

Figure S10. Frequency sweeps of a) Fe-Hpdca-PBCA and b) Fe-pdca-PBCA were performed at 1 Hz with 1% strain. The samples were stored at ambient environment for several days and rheology properties were tested every 2 days.

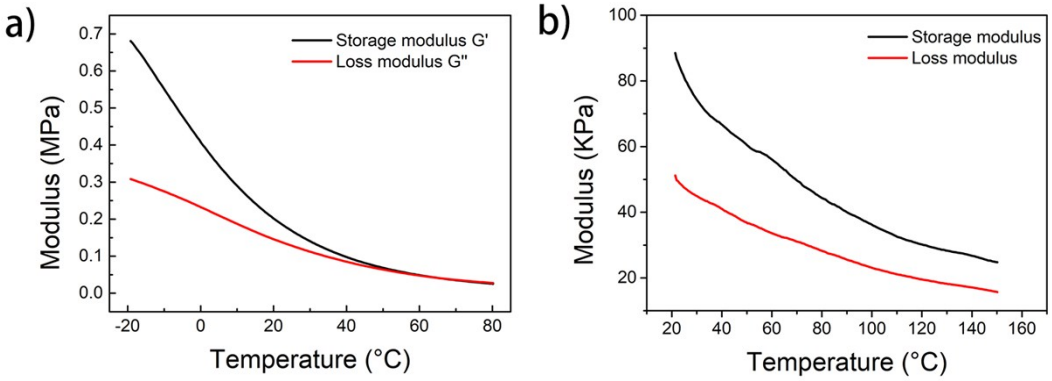

Figure S11. Oscillatory temperature ramps of a) Fe-Hpdca-PBCA and b) Fe-pdca-PBCA were performed at 1 Hz with a constant 1% strain.

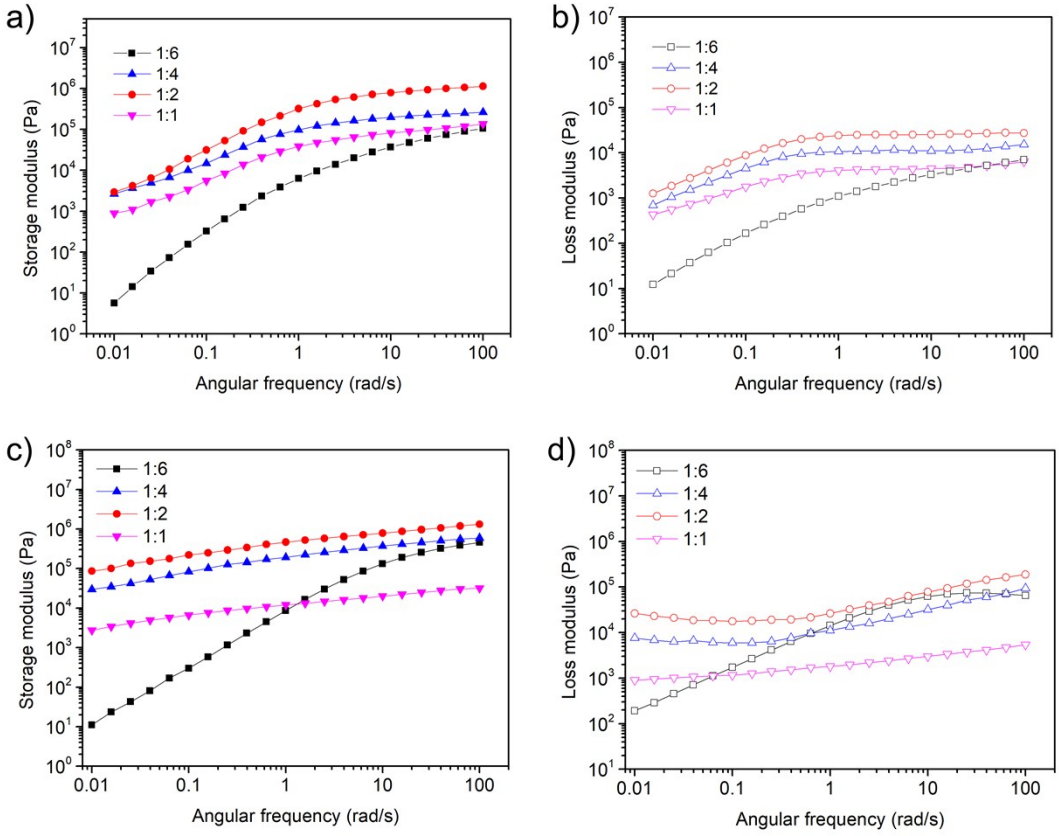

Figure S12. Rheology studies of Fe-Hpdca-PBCA ((a) Storage modulus and (b) Loss modulus) and Fe-pdca-PBCA ((c) Storage modulus and (d) Loss modulus) with different Fe(III) to ligand molar ratios.

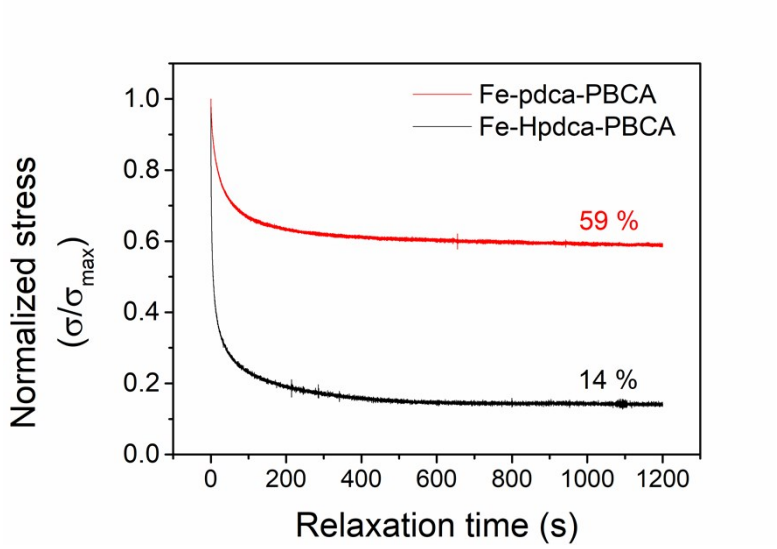

Figure S13. Stress-relaxation curves of Fe-Hpdca-PBCA and Fe-pdca-PBCA polymer films. The polymer films were primarily stretched to 40% strain, and then were allowed to relax for 1200 s at room temperature.

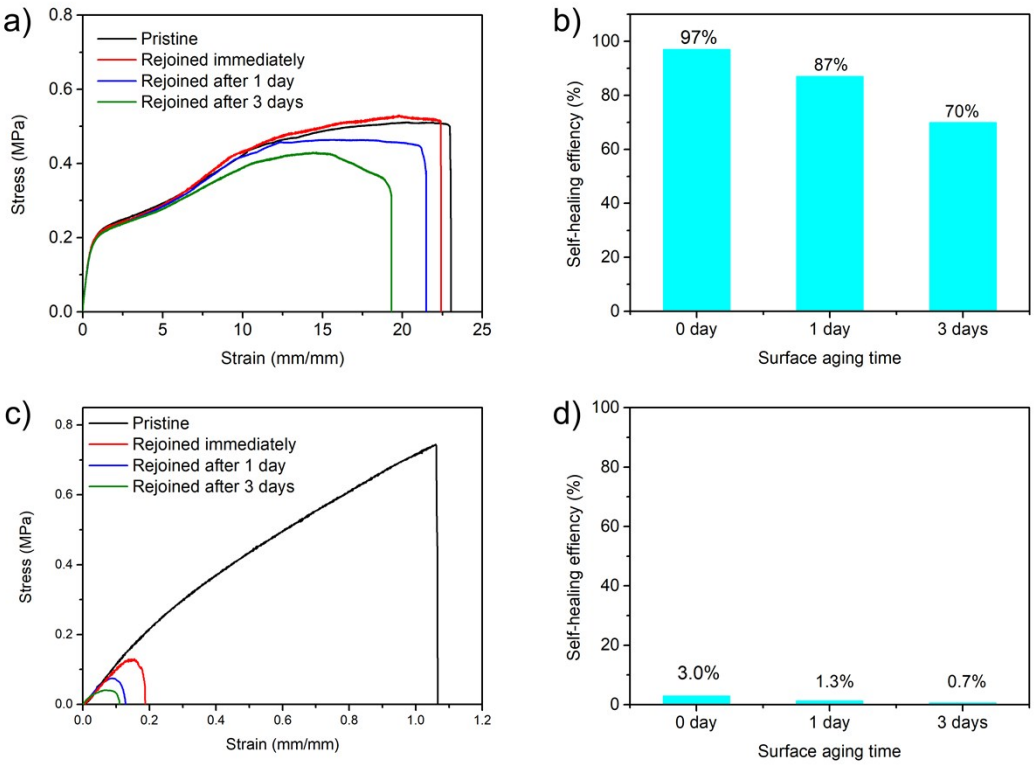

Figure S14. Self-healing properties of a) Fe-Hpdca-PBCA and b) Fe-pdca-PBCA with different surface aging time. All samples were put in ambient environment for different time after been cut, and then were allowed to rejoined together to heal at room temperature for 48 hours.